Amendments to the Claims:

This listing of claims will replace all prior versions and listings of claims in the application.

Listing of Claims:

1(currently amended). A computer-based method of generating a quantitative structure activity relationship, comprising:

a) calculating a numerical representation of molecules consisting of *n* numbers per molecule, ***n* being the number of molecular descriptors used to represent a molecule, and the molecule being a chemical compound**; ~~and,~~

b) estimating a probability distribution that **the *n* numbers of molecular descriptors were calculated from an active chemical compound, said probability distribution of said estimating step including the product of n one-dimensional distributions** ~~a said molecules is active~~ ;

c) using said probability distribution estimated in said estimating step to estimate the probability that a chemical compound is active against a particular biological target; and

d) displaying the probability that a chemical compound is active against a particular biological target to a user.

2(elected). A method as recited in claim 1, wherein:

a) said estimating step is calculated with Bayes Theorem.

3(cancelled).

4(withdrawn). A method as recited in claim 1, wherein:

a) said estimating step is performed by using a means to remove linear correlations between said *n* numbers per molecule.

5(withdrawn). A method as recited in claim 4, wherein:

a) said means to remove linear correlations between said *n* numbers per molecule is a principal components analysis.

6(withdrawn). A method as recited in claim 4, wherein:

a) said means to remove linear correlations between said *n* numbers per molecule is a matrix diagonalization.

7(withdrawn). A method as recited in claim 1, wherein:

a) said estimating step is performed by using a means to remove dependencies between said *n* numbers per molecule.

8(withdrawn). A method as recited in claim 7, wherein:

a) said means to remove dependencies between said *n* numbers per molecule is a principal components analysis.

9(withdrawn). A method as recited in claim 7, wherein:

a) said means to remove dependencies between said *n* numbers per molecule is a matrix diagonalization.

10(withdrawn). A method as recited in claim 1, wherein:

a) said estimating step is performed by estimating a distribution over a single number.

11(withdrawn). A method as recited in claim 1, wherein:

a) said estimating step is performed by replacing a single observation with a Gaussian distribution.

12(new). A computer-based method for developing a quantitative structure activity relationship, comprising:

a) obtaining a training set of chemical compounds with molecular descriptors including a number of multidimensional vectors with an activity class for each of said vectors;

b) partitioning said multidimensional vectors into groups, the groups having size one;

c) estimating a probability distribution of said descriptors by assuming that a probability distribution of a product of each of said groups of size one is approximately equal to said probability distribution of said multidimensional vectors;

d) performing said partitioning and estimating steps for each of said activity classes;

e) developing a probability distribution for said activity classes;

f) providing a particular biological target;

g) using the probability distribution to develop a quantitative structure activity relationship for interaction between the particular biological target and at least one of said activity classes of the training set of chemical compounds; and

h) displaying the probability that a chemical compound is active against a particular biological target to a user.

13. A computer-based method as recited in claim 12, wherein:

a) said training set of chemical compounds is obtained from high throughput screening data.

14. A computer-based method as recited in claim 12, wherein:

a) said training set of chemical compounds is comprised of virtual data.

15. A computer-based method as recited in claim 12, wherein:

a) said developing step is calculated with Bayes Theorem.